

Curriculum Vitae

Contact Address: :

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PERSONAL:

Name : : Prasenjit Seal
Father's Name : : Sri Pranab Kumar Seal
Date of Birth : : 26.02.1982
Nationality : : Indian
Sex : : Male
Marital Status : : Single

QUALIFICATION:

1st Class B.Sc. from University of Calcutta with Chemistry as Major.

(Year of Passing: 2003)

1st Class M.Sc. in Chemistry from University of Calcutta with Physical Chemistry as specialization.

(Year of Passing: 2005)

PhD in Science from University of Calcutta in the field of Theoretical Chemistry.

(Year of receiving degree: 2010)

PRESENT POSITION:

Post-Doctoral Research Fellow, Cristallographie, Résonance Magnétique et Modélisations (CRM2), Université Henri Poincare - Nancy 1, France.

AFFILIATION:

CRM2, Université Henri Poincaré - Nancy 1

Boulevard des Aiguillettes

B.P. 239

F-54506 Vandoeuvre-les-Nancy, France

DETAILS OF EDUCATIONAL QUALIFICATIONS:

Degree	Institution/Board/ University	Year	Percentage of marks & Division/Class
10 th Standard	Council for the Indian School Certificate Examinations, New Delhi	1998	79.5%
12 th Standard	West Bengal Council of Higher Secondary Education	2000	78.1%
B.Sc. (Hons. in Chemistry)	University of Calcutta	2003	64.875% 1 st Class
M.Sc. (Chemistry; specialization in Physical Chemistry)	University of Calcutta	2005	64.3% 1 st Class
PhD (Science)	University of Calcutta	2005-2009	

RESEARCH EXPERIENCE:

1. Doctoral research work under Dr. Swapan Chakrabarti, Department of Chemistry (Physical Chemistry section), University of Calcutta (5th September 2005 – 31st August, 2009).
2. Post-doctoral research work with Prof. János G. Ángyán, CRM2, Université Henri Poincaré – Nancy 1, France (1st December, 2009 – 31st March, 2011).

FIELD OF RESEARCH DURING Ph.D. TENURE:

Theoretical and Computational Chemistry.

In my Ph. D. tenure, I engaged myself in the following fields.

1. Linear and Nonlinear Response Properties of various molecules and small cluster materials.
2. Magnetic Properties of diradicals and dehydrogenated DNA base pairs.
3. Weak Interactions in benzene dimer, CH/ π interacting systems and rare gas-CO₂ complexes.
4. Explicit role of electron correlations in small carbon clusters and carbenes.
5. Relativistic Effect in atomic gold chain.
6. Aromaticity in several six-membered and four-membered heteroatomic systems.
7. Stability of certain systems.

FIELD OF RESEARCH DURING POST-DOCTORAL TENURE:

Range-Separated Density Functional Theory (RSH-DFT) along with the application of Random Phase Approximation (RPA) technique.

I am involved in benchmarking the performance of the RSH technique along with the RPA approach in various categories of weak-interacting systems. I am also involved in a project which deals with the estimation of Resta Localization Index, a field which is quite popular among physicists and slowly gaining importance within the chemistry community. Our group is involved in the development of the RSH-DFT approach and the scheme that we follow is implemented in the developing version of MOLPRO.

TITLE OF THESIS:

ELECTRONIC STRUCTURE CALCULATIONS OF SOME MOLECULES AND SMALL CLUSTERS WITH SPECIAL EMPHASIS ON OPTICAL AND MAGNETIC PROPERTIES

METHODS IMPLEMENTED DURING DOCTORAL STUDY:

Density Functional Theory (DFT) including time dependent case, Møller-Plesset perturbation theory, Configuration Interaction.

QUANTUM CHEMICAL SOFTWARES USED:

Gaussian 03, Amsterdam Density Functional (ADF), ORCA, DALTON, GAMESS, MOLPRO, dgrid, Bader Charge Analysis.

OTHER EXPERIENCES:

1. Well accustomed with FORTRAN (F77, F90 and F95).
2. Skill in using MATHEMATICA.
3. Familiar with both WINDOWS and LINUX environments.

REFERENCES:

❖ **Prof. Debashis Mukherjee**

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Indian Association for the Cultivation of Science
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❖ **Prof. János G. Ángyán**

Directeur de Recherches au CNRS
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❖ **Dr. Swapan Chakrabarti**

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List of publications/communications

1. “Explicit role of dynamical and nondynamical electron correlations on broken symmetry in C_{4N+2} clusters” by S. Sen, **P. Seal**, and S. Chakrabarti, *Phys. Rev. B* **73**, 245401 (2006).
2. “Explicit role of dynamical and nondynamical electron correlation on singlet–triplet splitting in carbenes”, by **P. Seal** and S. Chakrabarti, *Chem. Phys.* **332**, 232 (2007).
3. “Origin of the Nonplanarity of Tetrafluoro Cyclobutadiene, C_4F_4 ” by **P. Seal** and S. Chakrabarti, *J. Phys. Chem. A* **111**, 715 (2007).
4. “Reply to “Comment ‘Origin of the Nonplanarity of Tetrafluoro Cyclobutadiene, C_4F_4 ’”” by **P. Seal** and S. Chakrabarti, *J. Phys. Chem. A* **111**, 5119 (2007).
5. “Scalar relativistic effect on lattice dimerization in metastable gold nanowire of finite length” by **P. Seal** and S. Chakrabarti, *Chem. Phys.* **335**, 201 (2007).
6. “Is Nucleus-Independent Chemical Shift Scan a Reliable Aromaticity Index for Planar Heteroatomic Ring Systems?” by **P. Seal** and S. Chakrabarti, *J. Phys. Chem. A* **111**, 9988 (2007).
7. “Static and dynamic hyperpolarizability tensors of aluminum metal clusters, Al_4M_4 ($M = Li, Na, \text{ and } K$)” by S. Sen, **P. Seal**, and S. Chakrabarti, *Phys. Rev. B* **76**, 115414 (2007) * *Virtual Journal of Nanoscale Science & Technology*--- September 24, 2007 Volume 14, Issue 24).
8. “ $Si_xC_{1-x}O_2$ alloys: a possible route to stabilize carbon-based silica-like solids?” by Assa Aravindh, Artoto Arkundato, Sonali Barman, Stefano Baroni, Bhargava B.L., K.R.S. Chandrakumar, Wei Chen, Roby Cherian, Andrea Dal Corso, Soumendu Datta, Stefano de Gironcoli, Suman S. Dhayal, Alok Kumar Dixit, Sudipta Dutta, Pavel D'yachkov, Calin Gabriel Floare, Nirmal Ganguli, Shreemoyee Ganguly, Ralph Gebauer, Saurabh Ghosh, Paolo Giannozzi, Govind, Alison J. Hatt, Hembram K.P.S.S, Mighfar Imam, V. Jayalakshmi, C.S. Jayanthi, Tuhina Kelkar, Anil Kumar, Jun Hee Lee, Mal-Soon Lee, Dayana Lonappan, Priya Mahadevan, Sairam Swaroop Mallajosyula, Madhura Marathe, Nicola Marzari, Brent Melot, Nicholas Miller, Joseph Morrone, Sachin Nanavati, Asiri Nanayakkara, Prithwish Kumar Nandi, Shobhana Narasimhan(*), Bhaarati Natarajan, Fahmida Parvin, Sujata Paul, Kalpataru Pradhan, G. Praveena, Dasari L.V.K. Prasad, Himanshu K. Poswal, Bhalchandra Pujari, Raghani Pushpa, K. Hari Krishna Reddy, Srijan Kumar Saha, Carlo Sbraccia, Sandro Scandolo, **Prasenjit Seal**, Ghazal S. Shafai, Shanavas K.V., James O.H. Simrall, Aarti Srirangarajan, Vipul Srivastava, Mina K. Talati, Yuthana Tantirungrotechai, Kartick Tarafder, Tiju Thomas, and T. Uthayathan, *Solid State Communications* **144**, 273 (2007). [Done in a workshop]

9. "Static first order hyperpolarizabilities of DNA base pairs: A configuration interaction study" by **P. Seal**, P. C. Jha and S. Chakrabarti, *J. Mol. Struct.(THEOCHEM)* **855**, 64 (2008).
10. "Searching of potential energy curves for the benzene dimer using dispersion corrected density functional theory" by P. C. Jha, Z. Rinkevicius, H. Ågren, **P. Seal** and S. Chakrabarti, *Phys. Chem. Chem. Phys.* **10**, 2715 (2008).
11. "Magnetic Interactions in Alkyl Substituted Cyclohexane Diradical Systems: A Broken Symmetry Approach" by **P. Seal** and S. Chakrabarti, *J. Phys. Chem. A* **112**, 3409 (2008).
12. "Magnetic Interactions in Dehydrogenated Guanine-Cytosine (G-C) Base Pairs" by **P. Seal**, P. C. Jha, H. Ågren and S. Chakrabarti, *Chem. Phys. Lett.* **465**, 285 (2008).
13. "Static and dynamic polarizabilities of $(\text{CdSe})_n$ ($n=1-16$) clusters" by P. C. Jha, **P. Seal**, S. Sen, H. Ågren and S. Chakrabarti, *Comp. Mat. Sci.* **44**, 728 (2008).
14. "Is nucleus independent chemical shift scan can be used as a reliable aromaticity index for planar and neutral A_2B_2 clusters?" by **P. Seal**, *J. Mol. Struct. (THEOCHEM)* **893**, 31(2009).
15. "Suitability of Double Hybrid Density Functionals and Their Dispersion-Corrected Counterparts in Explaining the Potential Energy Curves for $\text{CO}_2 - \text{Rg}$ (Rg : He, Ne, Ar and Kr) Systems" by **P. Seal** and S. Chakrabarti, *J. Phys. Chem. A* **113**, 1377 (2009).
16. "CH/ π Interaction in Benzene and Substituted Derivatives with Halomethane: A Combined Density Functional and Dispersion-Corrected Density Functional Study" by R. C. Dey, **P. Seal**, and S. Chakrabarti, *J. Phys. Chem. A* **113**, 10113 (2009).
17. "Static First Order Nonlinear Optical Tensors of Alkali Metal Doped Linear $(\text{HCN})_n$ Clusters: A Configuration Interaction Study" by **P. Seal** and S. Chakrabarti, accepted, *Computing Lett. (CoLe)* (2009).
18. "Nonlinear Optical Switching Properties in the Furylfulgide Aberchrome 540-Dihydrobenzofuran Derivative Pair of Photochromic Materials" by **P. Seal** and S. Chakrabarti, *J. Phys. Chem. A* **114**, 673 (2010).
19. "Role of π -Conjugation in Influencing the Magnetic Interactions in Dinitrenes: A Broken-Symmetry Approach" by R. Ghosh, **P. Seal**, and S. Chakrabarti, *J. Phys. Chem. A* **114**, 93 (2010).

20. "Ab initio investigation on the nonlinear optical properties of Cd_nTe_n ($n=1-10$) clusters" by **P. Seal**, S. Sen, and S. Chakrabarti, *Chem. Phys.* **367**, 152 (2010).
21. "Carbondioxide Rare-Gas Systems: Sensitivity of Basis Sets and Double-Hybrid Density Functionals" by **P. Seal**, *J. Comput. Chem.* **31**, 2001 (2010).
22. "A Comparative Study of the Nonlinear Optical Properties of Cd_nX_n (X: S, Se and Te) Clusters" by S. Sen, **P. Seal**, and S. Chakrabarti, web publication on 27th July, *J. Cluster Sci.* (2010).
23. "Rationalizing the Aromaticity Indexes Used to Describe the Aromatic Behavior of Metal Clusters" by **P. Seal** and S. Chakrabarti in the book entitled "Aromaticity and Metal Clusters" edited by P. K. Chattaraj, Taylor and Francis (2010).
24. "Resta index, a global measure of delocalization of electrons: Theory vs experiment" by **P. Seal** and J. G. Ángyán, manuscript in preparation (2010).
25. "Asymptotic behavior of RSH+RPA interaction energies" by **P. Seal**, R. -F. Liu, J. G. Ángyán et al., manuscript in preparation (2010).
26. "Performance of range-separated hybrid schemes to model weak-interacting systems" by **P. Seal**, J. G. Ángyán et al., work in progress (2010).

Seminars/ Workshops/Conferences attended

- 1.** SERC School on Condensed Matter Physics at Saha Institute of Nuclear Physics, Kolkata (2nd January – 31st January, 2006).
- 2.** Discussion Meeting on Materials and Molecular Modelling at the Indian Association for the Cultivation of Science, Kolkata (8th March – 9th March, 2006).
- 3.** Summer School on Electronic Structure Methods and Applications, and Workshop on Computational Materials Theory at Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bangalore (10th July – 22nd July, 2006).
- 4.** International Seminar on Structure & Dynamics: from Micro to Macro 2006 at SINP auditorium, Kolkata (15th December – 17th December, 2006).
- 5.** School on Numerical Quantum Many-body Methods in Physics and Chemistry at Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bangalore (29th October – 3rd November, 2007).
- 6.** International Symposium on Atomic, Molecular and Optical Sciences: A Seamless Frontier at Vedic Village, Kolkata (10th January – 12th January, 2008).
- 7.** 2nd Workshop on High Performance Computing at the Indian Association for the Cultivation of Science, Kolkata (2nd April – 3rd April, 2008).
- 8.** International Symposium on Frontiers of Functional Materials at SINP auditorium, Kolkata (6th January – 7th January, 2009).
- 9.** Discussion Meeting on Theoretical Chemistry (TCS 2009) at Indian Institute of Science and Jawaharlal Nehru Center for Advanced Scientific Research (JNCASR), Bangalore (18th January – 22nd January, 2009).
- 10.** CECAM Workshop on vdW-DFT-RPA: "van der Waals forces in DFT, RPA and beyond" at Lausanne, Switzerland (28th June – 2nd July, 2010).

Fellowships, Awards and presentation

1. National Eligibility Test (NET) in 2004 and 2005 (qualified for the Shyma Prasad Mukherjee Fellowship).
2. Graduate Aptitude Test in Engineering (GATE) in 2005.
3. Oral presentation on “Explicit Role of Dynamic and Nondynamic Electron Correlation on C_{4N+2} Clusters” and Special reward certificate on basis of one of the best ten seminars cum active participation in SERC School on Condensed Matter Physics at Saha Institute of Nuclear Physics, Kolkata (2nd January – 31st January, 2006).
4. Poster presentation on “Can a cyclic homoatomic $4N\pi$ electronic system be aromatic?” at the International Seminar on Structure & Dynamics: from Micro to Macro 2006 at SINP auditorium, Kolkata (15th December – 17th December, 2006).
5. Poster presentation on “Benzene Dimer - Revisited” at School on Numerical Quantum Many-body Methods in Physics and Chemistry at Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bangalore (29th October – 3rd November, 2007).
6. Poster presentation on “Antiferromagnetic to Ferromagnetic transition in Guanine-Cytosine diradical: Role of weak interactions” at International Symposium on Atomic, Molecular and Optical Sciences: A Seamless Frontier at Vedic Village, Kolkata (10th January – 12th January, 2008).
7. Poster presentation on “ $(CdTe)_n$ Clusters: Materials with High NLO response” at the International Symposium on Frontiers of Functional Materials at SINP auditorium, Kolkata (6th January – 7th January, 2009).
8. Poster presentation on “Weak Interactions in $CO_2 - Rg$ (Rg: He, Ne, Ar and Kr) Systems: Suitability of DHDF and DHDF-D” at Discussion Meeting on Theoretical School Chemistry jointly organized by Indian Institute of Science and Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bangalore (18th January – 22nd January, 2009).
9. Joint winner of “Sir P. C. Ray Research Award” in Chemistry for the year 2008.
10. Poster presentation on “Description of Charge-Transfer (CT) System by Range-Separated Hybrid (RSH) Methods” at CECAM Workshop on vdW-DFT-RPA: "van der Waals forces in DFT, RPA and beyond" at Lausanne, Switzerland (28th June – 2nd July, 2010).